

Methanesulfonic acid
75-75-2 | DTXSID4026422

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.28×10^{-13} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.78×10^{-1}

Confidence level: 7.57×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Dimethyl sulfate

Measured: 5.00×10^{-13}

Predicted: 4.96×10^{-13}

Image not found

Methyl nitrite

Measured: 2.20×10^{-13}

Predicted: 2.32×10^{-13}

Image not found

Ethyl nitrate

Measured: 2.00×10^{-13}

Predicted: 3.49×10^{-13}

Image not found

Diethyl sulfate

Measured: 1.80×10^{-12}

Predicted: 1.55×10^{-12}

Image not found

Methyl nitrate

Measured: 3.50×10^{-13}

Predicted: 3.14×10^{-13}